

3,4-Dihydroxyacetophenone
1197-09-7 | DTXSID30152546

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.60e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.59e-01

Confidence level: 4.89e-01

Nearest Neighbors from the Training Set

Image not found

Tribromoacetic acid

Measured: 6.74e-01

Predicted: 5.34e-01

Image not found

Benzeneacetic acid, 4-hydroxy-

Measured: 3.99e-01

Predicted: 1.54e-01

Image not found

3-Hydroxyphenylacetic acid

Measured: 6.57

Predicted: 1.51e-01

Image not found

4-Hydroxybenzoic acid

Measured: 3.62e-02

Predicted: 9.91e-02